Truncation method for Green's functions in time-dependent fields

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Abstract

We investigate the influence of a time dependent, homogeneous electric field on scattering properties of non-interacting electrons in an arbitrary static potential. We develop a method to calculate the (Keldysh) Green's function in two complementary approaches. Starting from a plane wave basis, a formally exact solution is given in terms of the inverse of a matrix containing infinitely many 'photoblocks' which can be evaluated approximately by truncation. In the exact eigenstate basis of the scattering potential, we obtain a version of the Floquet state theory in the Green's functions language. The formalism is checked for cases such as a simple model of a double barrier in a strong electric field. Furthermore, an exact relation between the inelastic scattering rate due to the microwave and the AC conductivity of the system is derived which in particular holds near or at a metal–insulator transition in disordered systems.

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I. INTRODUCTION

The influence of a time-dependent electric field on properties of a quantum mechanical system is the topic of active recent research. An essential point in these investigations is that the time-dependent field is not from the beginning treated in perturbation theory (e.g. in linear response), but is rather considered as inherent part of the system itself. By this, one has to deal with conditions of a non-equilibrium situation under which the quantity of interest, e.g. a tunnel current or the response to an additional DC field, has to be determined. There is a considerable variety of physical systems studied so far. Many works are related to tunneling, such as driven quartic double wells [1], driven quantum wells [2] or tunneling through laser irradiated wells [3]. In interacting systems, investigations concentrated on tunneling through quantum dots in time-varying fields [4,5].

Another class of investigations are related to transport experiments as, e.g., in the quantum Hall regime [6–8], where a microwave gives rise to peculiar changes of the DC conductivities. Calculations have been done on photo-induced transport through quantum point contacts [9], or on microwave induced changes of the DC conductivity of a disordered system [10]. Recently, Holthaus and Hone [11] studied the Wannier-Stark ladder in an ac-driven one-dimensional tight- binding system, where in presence of disorder-induced localization the localization length is controlled by the time-dependent field.

In spite of this great variety of investigations, the main theoretical focus so far has been on the zero- or (quasi) one-dimensional case. It is therefore desirable to develop a calculation scheme that is applicable in higher dimensions and for arbitrary static potentials, in particular in view of applications as the quantum Hall effect ($d = 2$) or the Anderson transition ($d = 3$). In this paper, we set up a general formalism to calculate the Green's function of non–interacting electrons moving in an arbitrary static potential under the influence of a time–dependent electric field with frequency Ω. We use the Dyson equation to obtain the Keldysh Green's function in two different calculation schemes. First, we regard the static potential as a perturbation and include the electric field in the unperturbed Hamiltonian. We give a formally exact solution which can be evaluated approximately by inverting a truncated matrix containing a finite number of 'photo-blocks'. The advantage of this method is its exactness in the electric field; it furthermore sums up the static potential to infinite order and is perturbative in the higher *Fourier components* of the Green's function which correspond to the 'center–of–mass' time coordinate. Numerical examples of this 'truncation method' are presented for the trivial case of a constant potential, which allows comparison to an exact result, and a simple model for the transmission through a double barrier structure in a strong electric field. There, our method qualitatively reproduces previous results by other authors [12,3]. In particular, the examples show that already a small number of 'photo-blocks' is sufficient to obtain convergence.

Second, starting from the exact eigenstates of the static potential, again an exact formal solution is derived in which the Green's function is represented as the inverse of an infinite tridiagonal matrix, which is the Green's function analogue of the Floquet state Hamiltonian. This approach in particular is useful in situations where the static scattering problem is already solved (say by numerical diagonalization) and one is interested in the effect of an additional, time-dependent electric field. We calculate the electron self energy of which the diagonal part yields an inelastic scattering time τ_{MW} due to the influence of the electric

field. In the limit of $\hbar\Omega \ll E_F$ (where E_F is the Fermi level of the system without electric field) we obtain an exact relation between τ_{MW} and the zero temperature AC-conductivity of the system without electric field. We calculate τ_{MW} for microwave radiation in the integer quantum Hall effect. From the fact that τ_{MW} alone is insufficient to interpret experimental data, we conclude that one rather has to investigate the full Green's function in presence of the time–dependent electric field.

The paper is organized as follows. In section II, we set up the general formalism (Dyson's equation), in section III we specify to the plane wave basis and derive the exact expression for the Green's function which is evaluated numerically. In section IV, we give a formulation in the eigenstate basis of the static potential and discuss the electric field induced scattering rate, which again is derived from the formally exact result. A short conclusion is given in section V.

II. GENERAL FORMULATION

A. Dyson equation

The starting point in each of our approaches is the Dyson equation for the Keldysh Green's function matrices. We start from a basis of eigenstates labeled with α and define Green's functions [13] $iG_{\alpha\beta}^T(t_1, t_2) := \langle T c_\alpha(t_1) c_\beta^\dagger(t_2) \rangle$, $iG_{\alpha\beta}^{\tilde{T}}(t_1, t_2) := \langle \tilde{T} c_\alpha(t_1) c_\beta^\dagger(t_2) \rangle$, $iG_{\alpha\beta}^>(t_1, t_2) := \langle c_\alpha(t_1) c_\beta^\dagger(t_2) \rangle$, $iG_{\alpha\beta}^<(t_1, t_2) := -\langle c_\beta^\dagger(t_2) c_\alpha(t_1) \rangle$, where T ($\tilde{T}$) denote (anti)-chronological time ordering. Furthermore, the brackets $\langle \rangle$ denote as usual an average over a quantum state of the system (not necessarily the stationary state). The Green's functions are written in a matrix block

$$G(t_1, t_2) = \begin{pmatrix} G^T(t_1, t_2) & -G^<(t_1, t_2) \\ G^>(t_1, t_2) & -G^{\tilde{T}}(t_1, t_2) \end{pmatrix}, \tag{1}$$

for which the Dyson-integral equation has the same form as in equilibrium theory,

$$G(t_1, t_2) = G^0(t_1, t_2) + \int \int dt dt' G^0(t_1, t) \Sigma(t, t') G(t', t_2), \tag{2}$$

where the matrix Σ is composed of Σ^T, $-\Sigma^{\tilde{T}}$, $\Sigma^>$, $-\Sigma^<$, in analogy to Eq. (1). Here, G^0 denotes the unperturbed Greens' function, e.g. $iG_{\alpha\beta}^{T,0}(t_1, t_2) := \langle T \hat{c}_\alpha(t_1) \hat{c}_\beta^\dagger(t_2) \rangle$, where the electron creation (annihilation) operators $\hat{c}_\alpha^{(\dagger)}(t)$ are given in the interaction picture which will be defined according to the splitting of the total time dependent Hamiltonian $H(t)$. This splitting defines the way the perturbation theory is performed and will be explained below.

Since we are interested in a Hamiltonian a part of which oscillates with frequency Ω, it is useful to perform a Fourier analysis according to time 'center of mass' and relative coordinates ("Wigner–coordinates"), namely $T = (t_1 + t_2)/2$ and $t = t_1 - t_2$. This decomposition is defined according to

$$G(t_1 = T + t/2, t_2 = T - t/2) = \frac{1}{2\pi} \sum_N \int_{-\infty}^{\infty} d\omega e^{-i\omega t} e^{i\Omega N T} G(\omega, N) \tag{3}$$

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and correspondingly for G^0 and Σ. The inverse transformation is

$$G(\omega, N) = \int_{-\infty}^{\infty} dt e^{i\omega t} \int_0^{2\pi} \frac{d(\Omega T)}{2\pi} e^{-i\Omega N T} G(t_1 = T + t/2, t_2 = T - t/2). \tag{4}$$

Of special interest is the component $N = 0$ which determines the average over the 'center-of-mass' coordinate T. In particular, in the case of an equilibrium situation (no electric field), all components $G(\omega, N)$ with $N \neq 0$ vanish because the Green's function depends on the relative coordinate $t = t_1 - t_2$ only.

Inserting Eq. (3) into the Dyson equation Eq. (2), a straightforward calculation yields

$$G(\omega, N) = G^0(\omega, N) + \sum_{N_1 N_2} G^0\left(\omega + \frac{N_1 - N}{2}\Omega, N_1\right) \Sigma\left(\omega + \frac{N_1 - N_2}{2}\Omega, N - N_1 - N_2\right)$$
$$\times G\left(\omega + \frac{N - N_2}{2}\Omega, N_2\right). \tag{5}$$

In this paper, we concentrate on the non- interacting case where the perturbation is a one-particle operator and the self energy is (Keldysh) block-diagonal [14]

$$\Sigma(t, t') = \begin{pmatrix} V(t) & 0 \\ 0 & V(t) \end{pmatrix} \delta(t - t'). \tag{6}$$

An impurity average effectively introduces interactions among the electrons and the self energy becomes different from Eq. (6). However, as long as no impurity average is performed, one merely has to deal with a one- particle problem and the integral equation Eq. (2) together with Eq. (6) exactly determines the Green's function $G(t_1, t_2)$.

Because of the linear relation $G^T + G^{\tilde{T}} = G^> + G^<$, a rotation to tridiagonal form can be performed in Eq. (2). One of the resulting equations will be used later, namely the one for the retarded Green's function $iG^R_{\alpha\beta}(t_1, t_2) := \theta(t_1 - t_2)\langle c_\alpha(t_1)c_\beta^\dagger(t_2) + c_\beta^\dagger(t_2)c_\alpha(t_1)\rangle$, which reads, using $\Sigma^R(t, t') = V(t)\delta(t - t')$,

$$G^R(t_1, t_2) = G^{0,R}(t_1, t_2) + \int dt G^{0,R}(t_1, t)V(t)G^R(t, t_2). \tag{7}$$

B. Time-dependent field

In all what follows we assume that the system is subject to a spatially homogeneous electric field which oscillates in time with a frequency Ω and is polarized in direction $\mathbf{e}$,

$$\mathbf{E}(t) \equiv \mathbf{e}E_0 \cos(\Omega t). \tag{8}$$

The associated vector potential $\mathbf{A}^e(t) = -(\mathbf{e}E_0/\Omega)\sin(\Omega t)$ couples to the momentum $\mathbf{p}_i$ of the i-th electron via $\mathbf{p}_i \to \mathbf{p}_i - \mathbf{A}(\mathbf{x_i}) - \mathbf{A}^e(t)$, where $\mathbf{A}(\mathbf{x_i})$ is included here to indicate that there can be other contributions to the vector potential, e.g from a static magnetic field (we use units $\hbar = e = c = 1$ throughout). The *additional* energy through the electric field is

$$H_e(t) = \frac{E_0}{\Omega}\sin(\Omega t)\sum_{i=1}^{N_e}\mathbf{e}\mathbf{v}_i + N_e\Delta\Phi(t), \quad \Delta\Phi(t) := \frac{1}{2m^*\Omega^2}E_0^2\sin^2(\Omega t), \tag{9}$$

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where m^* is the bandmass, $m^* \mathbf{v_i} = \mathbf{p_i} - \mathbf{A}(\mathbf{x_i})$, and N_e the number of electrons in the system. We explicitly note that although the electric field $\mathbf{E}(t)$ is homogeneous, in an alternative gauge a corresponding *scalar potential* would be linear in the space coordinate, namely $\sim \mathbf{ex}\cos(\Omega t)$, an 'oscillating slanted surface'.

By gauge invariance, the current density operator is $\mathbf{j}(\mathbf{x},t) = \mathbf{j}_0(\mathbf{x}) - \frac{1}{m^*}\mathbf{A}^e(t)\rho(\mathbf{x})$, where $\mathbf{j}_0$ is the (paramagnetic) current density operator in the absence of the electric field, and $\rho(\mathbf{x})$ the electronic density.

In second quantization and in an basis of eigenstates $\{|\alpha\rangle\}$ with eigenenergies ε_α, the electric field gives rise to an additional Hamiltonian

$$H_e(t) = \frac{E_0}{\Omega}\sin(\Omega t)\sum_{\alpha\beta}\langle\alpha|v|\beta\rangle c_\alpha^\dagger c_\beta + \hat{N}\Delta\Phi(t). \tag{10}$$

Here, $v = (1/m^*)\mathbf{e}(\mathbf{p} - \mathbf{A}(\mathbf{x}))$ is the component of the electron velocity operator in direction $\mathbf{e}$. Note that the coupling is effectively to the velocity and not to the current density operator since we assumed spatial homogeneity of the electric field.

Care has to be taken when calculating Green's functions in a specific gauge, as has been pointed out by Bertoncini and Jauho [15]. Since only gauge-invariant quantities are meaningful for comparison with experiments, one has to formulate a gauge-invariant theory. In fact, a version $\tilde{G}$ of the Green's function which is invariant under a gauge transformation of the electric field can be recovered from the Green's function G in any specific gauge. In real space, this transformation is as follows [15]: if $\mathbf{R} = (\mathbf{x} + \mathbf{x}')/2$ and $\mathbf{r} = \mathbf{x} - \mathbf{x}'$ denote center-of mass and relative coordinates in real space and $t = t_1 - t_2$ and $T = (t_1 + t_2)/2$ the Wigner time variables,

$$\tilde{G}(\mathbf{r},t,\mathbf{R},T) = \exp\left(iw(\mathbf{r},t,\mathbf{R},T)\right)G(\mathbf{r},t,\mathbf{R},T), \tag{11}$$

where

$$w(\mathbf{r},t,\mathbf{R},T) := \int_{-1/2}^{1/2}d\lambda\left[\phi(\mathbf{R}+\lambda\mathbf{r},T+\lambda t) - \mathbf{r}\mathbf{A}^e(\mathbf{R}+\lambda\mathbf{r},T+\lambda t)\right], \tag{12}$$

and ϕ and $\mathbf{A}^e$ denote the static and the vector potential, respectively. Eq. (11) can be proofed directly by performing a gauge transformation $\mathbf{A}^e \to \mathbf{A}^e + \nabla\chi$, $\phi \to \phi - \partial_t\chi$ and using the fact that the field operators in real space transform as $\Psi \to \exp(i\chi)\Psi$ (note that we have set $e = \hbar = c = 1$). The factor $\exp(iw)$ becomes particularily simple in our case of a spacially homogeneous electric field defined through $\phi = 0$ and $\mathbf{A}^e(t) = -(\mathbf{e}E_0/\Omega)\sin(\Omega t)$. If we start in an arbitrary basis $\{|\alpha\rangle\}$ with wave functions $\Psi_\alpha(\mathbf{x})$, the gauge invariant object is

$$\tilde{G}(\mathbf{r},t,\mathbf{R},T) = \sum_{\alpha\beta}\Psi_\alpha(\mathbf{R}+\mathbf{r}/\mathbf{2})\Psi_\beta^*(\mathbf{R}-\mathbf{r}/\mathbf{2})\exp\left(iw(\mathbf{r},t,\mathbf{R},T)\right)G_{\alpha\beta}^\Phi(t,T), \tag{13}$$

where $G_{\alpha\beta}^\Phi(t,T)$ is calculated in a specific gauge and basis $|\alpha\rangle$.

In the rest of this paper, we will always refer to a specific gauge and refer to Eq. (13) for the final, gauge-invariant form. The importance of the phase factor $\exp(iw)$ depends on the physical situation and has been discussed, e.g., in [15,16]. For convenience, we split off another phase factor in Eq. (13). The last term in the Hamiltonian Eq. (10) which is

quadratic in E_0 couples to the total particle number operator $\hat{N}$ and thus gives rise to a phase factor in the Green's function. The latter can be written as

$$G^{\Phi}(t_1, t_2) = e^{i\Phi(t_1, t_2)} G(t_1, t_2), \quad \Phi(t_1, t_2) := N \int_{t_1}^{t_2} dt' \Delta\Phi(t'). \tag{14}$$

where N is the particle number and G the Green's function for the same Hamiltonian Eq. (10) but without the last term which, as can been directly seen from Eq. (10), shifts all energy levels ε_α by the same, but time dependent amount $\Delta\Phi(t)$.

III. PERTURBATION THEORY IN THE IMPURITY POTENTIAL

In the preceding section we have derived the general equation Eq. (5) which determines the Green's function of the system. As mentioned above, the splitting of the total Hamiltonian into perturbation part and unperturbed part defines the unperturbed Green's function G^0 which is at the base of any perturbation theory. In the following, we define the model Hamiltonian. In this section, we start from an eigenstate basis of plane waves, i.e. $|\alpha\rangle = |\mathbf{k}\rangle$ where $\langle \mathbf{x}|\mathbf{k}\rangle \equiv \phi_{\mathbf{k}}(\mathbf{x}) = (1/L^{d/2})\exp(-i\mathbf{k}\mathbf{x})$ and L^d is the system volume ($L \to \infty$ in the thermodynamic limit). We furthermore assume that there is no magnetic field, a non–zero magnetic field can be included in the basis of exact scattering states treated in the next section. In the plane wave basis, the velocity matrix element is diagonal,

$$\langle\alpha|v|\beta\rangle = \delta_{\alpha,\beta}\langle\alpha|v|\alpha\rangle \equiv \delta_{\alpha\beta}v_\alpha, \tag{15}$$

namely $v_\alpha = v_{\mathbf{k}} = \mathbf{e}\mathbf{k}/m^*$. Although Eq. (15) is exact only for plane waves, we keep the notation as general as possible and use greek letters labeling the eigenstates. The following results are then also valid for a general eigenstate basis with the approximation that non-diagonal elements of the velocity $\langle\alpha|v|\beta\rangle$ are zero. Because of Eq. (15), the Hamiltonian (system + electric field) is

$$H_0(t) = \sum_\alpha \varepsilon_\alpha(t) c_\alpha^\dagger c_\alpha; \quad \varepsilon_\alpha(t) \equiv \varepsilon_\alpha + \frac{E_0}{\Omega} v_\alpha \sin(\Omega t), \tag{16}$$

where ε_α is the energy of state α.

The static potential $V(\mathbf{x})$ now gives rise to an additional part to the total Hamiltonian which reads

$$H(t) = H_0(t) + V, \quad V = \sum_{\alpha\beta} V_{\alpha\beta} c_\alpha^\dagger c_\beta. \tag{17}$$

At this stage, V is not yet specified further. Depending on the physical situation, it describes a single impurity, a distribution of random scatterers, a double barrier etc. Note that according to the above, in Eq. (17) α denotes a plane wave while in the corresponding 'diagonal approximation' case for arbitrary basis α the potential term V does not appear and simply $H(t) = H_0(t)$.

A. Dyson equation in arbitrary strong electric fields

We define an interaction picture with respect to the unperturbed part H_0 of the Hamiltonian according to

$$\hat{c}_\alpha(t) = U_0^\dagger(t, t_0) c_\alpha U_0(t, t_0), \quad U_0(t, t_0) = T \exp\left(-i \int_{t_0}^t dt' H_0(t')\right). \tag{18}$$

The unperturbed time-ordered Green's function then is

$$iG_{\alpha\beta}^{T,0}(t_1, t_2) = \langle T \hat{c}_\alpha(t_1) \hat{c}_\beta^\dagger(t_2) \rangle =$$
$$= e^{-i \int_{t_2}^{t_1} dt' \varepsilon_\alpha(t')} \left[\theta(t_1 - t_2)(1 - f_\alpha) - \theta(t_2 - t_1) f_\alpha\right] \delta_{\alpha\beta}, \qquad f_\alpha = \langle c_\alpha^\dagger c_\alpha \rangle \tag{19}$$

and correspondingly for the other Green's functions. The average $\langle\rangle$ gives rise to a distribution function f_α which not necessarily coincides with the Fermi distribution. Note that the value of the fixed time t_0 in Eq. (18) is not relevant for G. The Green's function Eq. (19) can be related to the free ($V = 0$) Green's function without electric field ($E_0 = 0$), which in the following is called G^{free}. Namely, one has for the time-ordered part

$$G_{\alpha\beta}^{T,0}(t_1, t_2) = e^{ig_\alpha[\cos(\Omega t_1) - \cos(\Omega t_2)]} G_\alpha^{T,free}(t_1 - t_2)\delta_{\alpha\beta}, \qquad g_\alpha := \frac{E_0 v_\alpha}{\Omega^2} \tag{20}$$

and correspondingly for the other Keldysh-block components. The effect of the electric field thus is incorporated in the phase factor in front of $G^{T,free}$ in Eq. (20). Note that this phase factor, in contrast to the 'global' phase $\Phi(t_1, t_2)$, Eq. (14), depends on the quantum number α which will be important when scattering, i.e. transitions between different states $\alpha \to \beta$, is considered.

To get into contact with the Fourier representation above, we use a decomposition into Bessel functions according to $\exp[iz \cos(\Omega t)] = \sum_n i^n J_n(z) \exp(in\Omega t)$ (the sum is over all integers n). We obtain

$$G_{\alpha\beta}^0(\omega, N) = i^N \sum_n J_n(g_\alpha) J_{N-n}(-g_\alpha) G_\alpha^{free}(\omega + [n - N/2]\Omega)\delta_{\alpha\beta} \tag{21}$$

for the Keldysh Green's function matrix. Note that G^{free} depends on one Fourier variable only since the corresponding $G^{free}(t_1 - t_2)$ is a function of the time difference only. We note again that the eigenstate basis in this section consists of plane waves $|\alpha\rangle = |\mathbf{k}\rangle$ with momentum $\mathbf{k}$. Only in the 'diagonal approximation' model, where one neglects the potential term V in Eq. (17), the results of this section can be transfered to an arbitrary eigenstate basis. Furthermore, in this section G^0 denotes the Green's function belonging to the *time-dependent* Hamiltonian $H_0(t)$, Eq. (16). It contains the electric field exactly to all orders of the coupling parameter g_α, Eq. (20), which appears in the argument of the Bessel functions.

We now proceed to set up a systematic approximation scheme that allows to calculate the Fourier components $G_{\alpha\beta}(\omega, N)$ of the Green's function belonging to the time-dependent Hamiltonian $H(t)$, Eq. (17). In particular, the effect of the time dependent field will be fully incorporated through the unperturbed Green's functions G^0, Eq. (21).

Since the perturbation potential V is time-independent, the selfenergy in Eq. (5) is

$$\Sigma(\omega, N) = S \cdot \delta_{N,0}, \quad S = \begin{pmatrix} V & 0 \\ 0 & V \end{pmatrix}. \tag{22}$$

Thus,

$$G(\omega, N) = G^0(\omega, N) + \sum_{N_1} G^0\left(\omega + \frac{N_1 - N}{2}\Omega, N_1\right) SG\left(\omega + \frac{N_1}{2}\Omega, N - N_1\right). \tag{23}$$

One immediately sees the fundamental difficulty in Eq. (23): Even for obtaining only the Fourier component $G(\omega, N = 0)$, corresponding to an average of the 'center-of-mass' time coordinate, the N_1-sum couples the different N–components in Eq. (23).

An obvious approximation would be to neglect all $N \neq 0$ components at all, i.e. to neglect the center-of-mass time coordinate. Indeed, approximations of this kind have been used recently (we call it 'fast' approximation in the following), namely in the so-called 'non-adiabatic regime' of resonant tunneling [3] where the frequency Ω of the time dependent field is much larger than the inverse tunneling time. Another example is the neglect of higher order Fourier components in the calculation of Green's functions for Wannier Stark systems [11]. There, the approximations were argued to work well for frequencies Ω larger than the bandwidth of the systems (the letter is proportional to the hopping matrix element of the corresponding tight-binding Hamiltonian). The extreme advantage of those approximations is that in a relatively simple manner the effect of the time dependent field can be incorporated by essentially calculating expressions where the free Green's function $G^{free}(\omega)$ is replaced by $G^0(\omega, N = 0)$, Eq. (21).

In the general situation of an (arbitrary) disorder potential or an arbitrary eigenstate basis, it is not clear if an analogy to the fast approximation exists. Furthermore, the validity of the latter has not been investigated systematically to our knowledge. In the following, we develop a scheme for such an investigation. The formalism set up below is completely general and can be applied to a large range of other situations, too. This opens the possibility to go beyond the 'fast approximation' in a general scattering situation.

B. Fast approximation and its first corrections

We start calculating the $N = 0, \pm 1$ components of $G(\omega, N)$, Eq. (23), i.e. the 'fast' approximation which neglects the 'center–of–mass' time coordinate T, and its first corrections. Introducing the convenient notation

$$g_{l,n}^{(0)} := G^{(0)}\left(\omega + \frac{l}{2}\Omega, n\right), \tag{24}$$

we obtain from the terms $N_1 = 0, \pm 1$ in Eq. (23) the approximate solution

$$g_{l,n} \approx g_{ln}^0 + g_{l-n,0}^0 S g_{l,n} + g_{1+l-n,1}^0 S g_{1+l,n-1} + g_{-1+l-n,-1}^0 S g_{l-1,n+1}. \tag{25}$$

Here, all quantities are (Keldysh block-) matrices. The problem of determining the (time-average) component $g_{0,0} = G(\omega, N = 0)$ is pure algebra and one obtains

$$G(\omega, N = 0) \approx (1 - \tilde{g}^0 S)^{-1} \tilde{g}^0$$
$$\tilde{g}^0 = g_{0,0}^0 + g_{1,1}^0 S(1 - g_{2,0}^0 S)^{-1} g_{1,-1}^0 + g_{-1,-1}^0 S(1 - g_{-2,0}^0 S)^{-1} g_{-1,1}^0. \tag{26}$$

Equivalently, other components than $N = 0$ might be calculated. Note that Eq. (26) has the standard form of the formal solution of the time-independent Dyson equation for a self energy S (which for our case of a static potential V is given by V itself),

$$G(\omega) = (1 - G^{free}(\omega)S)^{-1}G^{free}(\omega). \tag{27}$$

However, the 'unperturbed' Green's function $g_{0,0}^0$ is substituted by the more complicated expression $\tilde{g}^0$. In fact, having $g_{0,0}^0$ instead of $\tilde{g}^0$ in Eq. (26) is exactly the 'fast approximation', namely

$$G(\omega, N = 0) \approx (1 - G^0(\omega, N = 0)S)^{-1}G^0(\omega, N = 0). \tag{28}$$

Eq. (28) is the zeroth order approximation for Eq. (23) with respect to the Fourier index N. In particular, the dependence on the 'center-of-mass' time coordinate T, Eq. (3) is completely neglected here.

C. Exact solution

The perturbative calculation of the $N = 0, \pm 1$–components of $G(\omega, N)$ above suggests that there is a general solution of the Dyson equation type which holds to all orders. Eq. (23) can be solved formally to *all orders* in the self energy and for all components N. The procedure for this is very similar to the derivation of the Floquet-matrix in the exact eigenstate basis below. Here, we derive the exact result in the plane wave basis. It is the generalization of the Dyson equation solution for a time–independent scattering problem to the case of an additional time-dependent electric field and will be the starting point for the subsequent numerical truncation scheme.

We first rewrite Eq. (23) as

$$g_{ln} = g_{ln}^0 + \sum_{n'} g_{l+n',n'+n}^0 S g_{l+n+n',-n'}, \tag{29}$$

where we shifted the n'-summation index. We introduce a matrix γ with elements $\gamma_{rs} = g_{ln} \equiv g_{r+s,s-r}$, together with a matrix γ^0 with the corresponding elements of g^0. We perform an index transformation

$$r = (l - n)/2, \quad s = (l + n)/2, \tag{30}$$

which yields

$$\gamma_{rs} = \gamma_{rs}^0 + \sum_{n'} \gamma_{rn'}^0 S \gamma_{n's}. \tag{31}$$

Therefore, in the space of the (r, s)-indices, the solution of the matrix equation becomes

$$\gamma = (1 - \gamma^0 S)^{-1}\gamma^0. \tag{32}$$

Explicitely, the matrix γ has the form

$$\gamma = \begin{pmatrix} \cdots & & & \\ & 1 - g^0_{-20}S & -g^0_{-11}S & -g^0_{02}S & \cdots \\ \cdots & -g^0_{-1-1}S & 1 - g^0_{00}S & -g^0_{11}S & \cdots \\ & -g^0_{0-2}S & -g^0_{1-1}S & 1 - g^0_{20}S & \cdots \\ \cdots & & & & \cdots \end{pmatrix}^{-1} \times \gamma^0. \tag{33}$$

In particular, the matrix $(1 - \gamma^0 S)$ is fully occupied.

Since γ is just another representation of the original matrix g, $\gamma_{rs} = g_{r+s,s-r}$, Eq. (33) solves the Dyson equation Eq. (23) exactly. Note that the elements of the matrix γ are (Keldysh) matrices themselves. This tensor structure is analogous to the formal solution in the exact eigenstate basis below, here we started from a plane wave eigenstate basis $|\mathbf{k}\rangle$. While γ^0 is diagonal in this basis, the self energy S in general is not diagonal and depends on k and k' for a given static potential.

In the usual time-independent case, solving the Dyson equation Eq. (27) for an arbitrary potential requires the inversion of a matrix of dimension D, where D is the dimension of the eigenstate basis (which is finite in any numerical calculation). In the present time-dependent case, the effective dimension of the matrix γ is D times n_{ph}, where n_{ph} is the number of 'photoblocks' in $(1 - \gamma^0 S)$, e.g. $n_{ph} = 3$ for the three blocks per row in Eq. (33). Since there are infinitely many Fourier components of the Green's function, in the exact solution Eq. (33), $n_{ph} = \infty$, and γ is of infinite dimension even if the dimension D of the original Hilbert space is finite. It turns out, however, that it is sufficient to consider only a relatively small number of these blocks in practical calculations. In principle, the numerical effort increases rapidly with the number n_{ph}. Fortunately, the examples below show that convergence is reached quickly by truncating γ at relatively small n_{ph}. We also stress that this 'truncation method' is to infinite order in the static potential V *and* the electric field E_0. It is perturbative in the higher *Fourier components* (large n) for the center–of–mass time coordinate T in g^0_{ln} in the off–diagonal in Eq. (33).

Since Eq. (33) is the exact solution of Eq. (23), one easily recovers the above approximations: The 'fast approximation' Eq. (28) is obtained by cutting the matrix $(1 - \gamma^0 S)$ such that only the $(r = 0, s = 0)$, i.e. the 'central' element is retained. In (r, s) space the (infinite) matrix becomes a number and the inversion is trivial. The next approximation Eq. (26) that retains only the $N = 0, \pm 1$ components can be verified similarly by inversion of the corresponding 3×3 matrix in (r, s)-space.

Eq. (33) offers the possibility of a systematic investigation of the 'truncation method', in particular of approximations like Eq. (26) or Eq. (28).

D. Numerical examples

In the following, we apply the formalism to calculate the *time-averaged* Green's function $G(\omega, N = 0)$ numerically, using Eq. (33) in two different potentials V.

1. Constant potential

In the first model, we use a constant self energy $V = const$. Physically, this is a trivial, nevertheless very instructive situation since it offers comparison to an exact solution. That

is, the constant shift of the energy scale by V corresponds to the exact result

$$G_k(\omega, N) = G_k^0(\omega - V, N) \tag{34}$$

which has to be reproduced by inverting the full Dyson equation, Eq. (33). Here, G_k^0 is the unperturbed ($V = 0$) Green's function defined according to Eq. (21).

The result of the numerical inversion is shown for the $N = 0$–component of the corresponding spectral function component which we defined from the Green's function as

$$A_k(\omega, N = 0) := -\frac{1}{\pi} \operatorname{Im} G_k^R(\omega, N = 0), \tag{35}$$

through the retarded Green's function. The numerical calculation here is regarded as a check for the consistency and convergence of the formalism as such. Therefore, for reasons of simplicity we did not calculate the full 'physical' spectral function $A_k(\omega)$ [16] which involves the additional phase factor w, Eq. (13). Note that because of Eq. (7), we only have to consider retarded functions in the Dyson equation. In particular, in our plane wave basis the elements $1 - G_{l,n}^0 S = 1 - G_{l,n}^0 V$ are (complex) numbers and not matrices since we are working in Fourier space and not in real space here.

The results of the numerical inversion of Eq. (33) are shown in Fig. (1) and Fig. (2). We fixed the wavevector $k = k_F$, energies are measured in units of the Fermi energy $E_F = (\hbar k_F)^2 / 2m^*$. The dimensionless parameter α regulating the coupling to the electric field of strength E_0 is defined as

$$\alpha = E_0 k_F / (m^* \Omega^2). \tag{36}$$

For a potential $V = 0.22 E_F$ and strong coupling, $\alpha = 2$, the central peak of the spectral function is strongly suppressed: its main weight comes from the Bessel functions J_0^2, on the other hand, the product αk is close to the first zero of the latter. Side-peaks appear at values of the energy ω shifted by multiples $n\Omega$. The exact result Eq. (34) is excellently reproduced by inversion of the 11×11 'photo'block matrix Eq. (33), while the 'fast approximation' Eq. (28) gives a totally wrong result. In contrast to this, already the inversion of the 5×5 matrix qualitatively reproduces the exact result. The situation is less dramatic for smaller coupling $\alpha = 0.5$ and smaller potential $V = 0.03 E_F$. There, the 'fast approximation' Eq. (28) is qualitatively roughly correct whereas the exact result is already obtained from the 5×5 matrix inverse.

2. Resonant tunneling

In the second example, we investigated a physically non-trivial situation, namely the transmission of an electron through a double-barrier structure. The model is a one-dimensional lattice with j_{max} sites and a potential

$$S = V = |x_1\rangle V_1 \langle x_1| + |x_2\rangle V_2 \langle x_2|. \tag{37}$$

For $V_1, V_2 > 0$, this potential has a resonant structure in its transmission coefficient and can be regarded as a simple version of a model simulating a quantum well double barrier.

The Dyson equation Eq. (23) has to be transformed to real space to obtain the matrix elements $\langle x|G(\omega, N)|x'\rangle$ of the full Green's function in real space. Changing from the original plane-wave basis to real space in particular involves a Fourier transformation in the Green's function G^0,

$$G^0(x - x'; \omega, N) = \frac{1}{2\pi} \int dk e^{ik(x-x')} G_k^0(\omega, N). \tag{38}$$

In fact, the integral Eq. (38) is tedious and we found an analytical form for the retarded Green's function only for small couplings $x_0 = E_0/m^*\Omega^2$, namely

$$G^{0,r}(x - x'; \omega, N) = [\text{sgn}(x - x')i]^N \sum_n J_n(x_0\sqrt{z}) J_{N-n}(-x_0\sqrt{z}) \frac{-i}{2\sqrt{z}} e^{i\sqrt{z}|x-x'|},$$
$$z := \omega + (n - N/2)\Omega, \quad 2x_0 < |x - x'| \tag{39}$$

For smaller $|x - x'|$, we resorted to a numerical evaluation of the integral. We defined the coefficient

$$T(\omega) := \left| \frac{G^r(x, x', \omega, N = 0)}{G^{0,r}(x - x', \omega, N = 0)} \right|^2 \tag{40}$$

from the time-averaged $N = 0$–components of the Green's functions which is independent of x, x' for $x < x_1$ and $x' > x_2$, i.e. transmission of an incoming electron (from left) through both potentials at sites x_1 and x_2. Strictly speaking, since $T(\omega)$ is defined by the product of the time-averaged G's and not the time-average of the product GG^*, $T(\omega)$ deviates from the (physical) time-averaged transmission coefficient. Here as above we restrict ourselves, however, to the simpler quantity Eq. (40) to clarify the convergence of the numerical method to determine G. We chose $j_{max} = 12$ and a distance $x_2 - x_1 = 2a$, where a is the lattice constant serving as length scale and $E_a = \hbar^2/2m^*a^2$ for the energy scale. The number n_{ph} of 'photo-blocks' in the matrix $(1 - \gamma^0 S)$ again determines the total size of the matrix to be inverted. Each block itself is a $j_{max} \times j_{max}$–matrix, the total dimension of the matrix therefore being $j_{max} \times n_{ph}$.

Fig. (3) shows the coefficient $T(\omega)$ for three different sizes of the matrix Eq. (33). One reckognizes that already for $n_{ph} = 5$ convergence is reached practically for all values of the energy ω. The side-peaks to the left and to the right of the transmission maximum correspond to the first 'side-bands' $\pm\hbar\Omega$ for tunneling through the double barrier and have been found previously by Iñarrea et al. [12].

We conclude that the numerical inversion of Eq. (33) shows the extremely good convergence of the results from truncating Eq. (33), in contrast to the approximation Eq. (28). This in particular indicates that one has to be very careful when using approximations where Fourier components of the Green's function are neglected. We rather believe that our calculation shows that in general one has to consider at least a certain number of components $G(\omega, N)$, $N \neq 0$, from the very beginning. In the original representation of $G(t_1, t_2)$, Eq. (3), this means that not only the relative time coordinate $t_1 - t_2$ but also the 'center-of-mass' time coordinate T is important.

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IV. TIME DEPENDENT FIELD AS PERTURBATION

The basic advantage of the above approach is its exactness to all orders in the electric field which *a priori* is incorporated in the free Green's function G^0. The exact result Eq. (33) implies that one solves the *static* scattering problem and the effect of the electric field simultaneously. By inverting the truncated matrix one sums up the static potential V to infinite order. Still, higher Fourier component terms Sg^0_{rs} proportional to V in the off-diagonal of Eq. (33) are neglected. On the other hand, there are situations where one wishes to make no approximations concerning the static potential, in particular in systems where localization plays a role. Furthermore, in cases where the static potential is complicated, practical calculations become tedious in the plane wave basis. In fact, if the static scattering problem is already solved (say by numerical diagonalization), the basis of the static potential eigenstates provides the ideal starting point.

In the following, we therefore take a different point of view and consider the electric field as a perturbation while starting from the exact basis of eigenstates of the system, i.e. the scattering states of the static potential V. In presence of an additional, static magnetic field $\mathbf{B}$, these are the scattering states of the static potential in presence of $\mathbf{B}$. As above, a formally exact expression for the Green's function is derived which is closely related to the Floquet state formalism [17]. As an application, we derive an exact expression for the dephasing time due to the time-dependent electric field expressed in terms of the AC-conductivity of the system in absence of the electric field. This expression in particular is valid near or at a metal-insulator transition.

We start from a Hamiltonian

$$H(t) = H_0 + M(t) = \sum_\alpha \varepsilon_\alpha c_\alpha^\dagger c_\alpha + \sum_{\alpha\beta} M_{\alpha\beta}(t) c_\alpha^\dagger c_\beta$$

$$M_{\alpha\beta}(t) = M_{\alpha\beta} \sin(\Omega t) = \frac{E_0}{\Omega} \langle \alpha|v|\beta \rangle \sin(\Omega t). \tag{41}$$

The unperturbed part H_0 is now time-independent and describes the non-interacting system in the exact eigenstate basis, labeled with the index α. An additional advantage is that the unperturbed quantities are now defined in an equilibrium system in contrast to the case in the preceding section. There, $H_0(t)$ was time dependent and thus even the unperturbed system not in equilibrium.

The matrix element $M_{\alpha\beta}$ describes transitions from states α to states β and couples to the velocity matrix element $\langle \alpha|v|\beta \rangle$ in polarization direction of the electric field. In Fourier representation, the free Green's function G^0 belonging to H_0 is diagonal and depends on the time difference only, while the self energy $\Sigma(t, t') = \delta(t - t') \sin(\Omega t)\Sigma$ has components $N = \pm 1$,

$$G^0_{\alpha\beta}(\omega, N) = \delta_{N,0}\delta_{\alpha\beta}G^0_\alpha(\omega)$$

$$\Sigma_{\alpha\beta}(\omega, N) = \Sigma_{\alpha\beta}[\delta_{N,1} - \delta_{N,-1}], \quad \Sigma_{\alpha\beta} \equiv \frac{1}{2i}W_{\alpha\beta} \equiv \frac{1}{2i} \begin{pmatrix} M_{\alpha\beta} & 0 \\ 0 & M_{\alpha\beta} \end{pmatrix}. \tag{42}$$

Using the general Eq. (5) one obtains

$$G(\omega, N) = G^0(\omega)\delta_{N,0} + G^0\left(\omega - \frac{N\Omega}{2}\right)\Sigma\left[G\left(\omega + \frac{\Omega}{2}, N - 1\right) - G\left(\omega - \frac{\Omega}{2}, N + 1\right)\right]. \tag{43}$$

For convenience, we again use the notation Eq. (24) $g_{l,n} = G(\omega + l\Omega/2, n)$, furthermore $g_l^0 = G^0(\omega + l\Omega/2)$, so that Eq. (43) becomes

$$g_{l,n} = \delta_{n,0}g_l^0 + g_{l-n}^0 \Sigma[g_{l+1,n-1} - g_{l-1,n+1}]. \tag{44}$$

We note that again all quantities are Keldysh block matrices, each block being a matrix in the indices α, β that label the *exact* eigenstates of H_0 (static scattering potential plus magnetic field). The free Green's function G^0 in this chapter thus refers to the time-independent part H_0 only and is diagonal in the eigenstate basis.

A. Exact formal solution

We use the index transformation Eq. (30) $r = (l-n)/2$, $s = (l+n)/2$, $r, s = 0, \pm1, \pm2, ...$ which allows for a formal solution of Eq. (44) and shows the relation to the Floquet state theory. Again, we define the matrices

$$\Gamma_{rs} := g_{r+s,s-r} \equiv g_{l,n}$$
$$\Gamma_{2r}^0 := g_{l-n}^0, \quad \Gamma_{rs}^0 := \delta_{rs}\Gamma_{2r}^0 = \delta_{n,0}g_l^0. \tag{45}$$

Note that in contrast to the previous section, Γ and g now refer to the exact eigenstate basis. The requirement that both r and s are integer numbers in fact restricts the value of l: Even $n = s - r$ requires even $l = s + r$ and odd n requires odd l. From the definition of $g_{ln} = G(\omega + l/2\Omega, n)$ one reckognizes, however, that the index l is redundant in the sense that *one* value of l is sufficient to obtain the full information of the function $G(\omega, n)$. This kind of redundance is well-known from the Floquet state formalism [17] to which the analogy becomes evident in the following.

From Eq. (44), we obtain a corresponding equation in the $r, s-$ space, using $g_{l\pm1,n\mp1} = \Gamma_{r\pm1,s}$,

$$\Gamma_{rs} = \Gamma_{rs}^0 + \Gamma_{2r}^0 \Sigma \left[\Gamma_{r+1,s} - \Gamma_{r-1,s}\right]. \tag{46}$$

After introducing

$$\sigma_{rr'} = (\delta_{r+1,r'} - \delta_{r-1,r'})\Sigma, \tag{47}$$

this can be written in the matrix form

$$\Gamma = \Gamma^0 + \Gamma^0 \sigma \Gamma = \left[(\Gamma^0)^{-1} - \sigma\right]^{-1}. \tag{48}$$

Eq. (48) is the formal solution of the problem to determine the Green's function for the Hamiltonian Eq. (41). The structure of the matrix Γ is as follows: Since Γ^0 is diagonal in r and s, one has $(\Gamma^0)_{rs}^{-1} = \delta_{rs}(g_{l=2r,n=0}^0)^{-1} = \delta_{rs}G^0(\omega + r\Omega)^{-1}$. Therefore, the matrix Γ is the inverse of a tridiagonal matrix,

$$\Gamma = \begin{pmatrix} \ddots & & & & \\ & G^0(\omega - \Omega)^{-1} & -\Sigma & & \mathbf{0} \\ & \Sigma & G^0(\omega)^{-1} & -\Sigma & \\ & & \Sigma & G^0(\omega + \Omega)^{-1} & -\Sigma \\ & \mathbf{0} & & \Sigma & G^0(\omega + 2\Omega)^{-1} & -\Sigma \\ & & & & \Sigma & \ddots \end{pmatrix}^{-1}, \tag{49}$$

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i.e. an infinite tridiagonal block matrix in the space of 'photon numbers'. Note that the elements of γ are (Keldysh) matrices themselves and in general infinite-dimensional as is the Hilbert space belonging to the Hamiltonian H_0.

To give an illustrative example, we consider a two-level system with energies ε_α and ε_β, coupled to a time-dependent field via the matrix element $M_{\alpha\beta} = M_{\beta\alpha} = 2b$, $M_{\alpha\alpha} = M_{\beta\beta} = 0$. Taking the limit $\omega \to 0$ in Eq. (49), we obtain (notice that the quantity Γ is just a representation of the Green's function G itself):

$$
- G^R(\omega \to 0) = \begin{pmatrix} \ddots & & & & & \\ & \Omega + \varepsilon_\alpha & 0 & 0 & -ib & \\ & 0 & \Omega + \varepsilon_\beta & -ib & 0 & \\ & 0 & ib & \varepsilon_\alpha & 0 & 0 \\ & ib & 0 & 0 & \varepsilon_\beta & -ib \\ & & & & & \ddots \end{pmatrix}^{-1} .
\tag{50}
$$

In the case of a coupling proportional to $\cos(\Omega t)$ instead of $\sin(\Omega t)$, one easily verifies that $\pm ib$ is replaced by b in Eq. (50). One then has exact coincidence with the formal solution of the time-dependent two-level problem first given by Shirley [17] in his seminal paper on the Floquet state theory. Here, we have reproduced those results in the language of Green's functions starting from the Dyson equation. The Floquet Hamiltonian $\mathcal{H}$ is obtained as the limit $\mathcal{H} = -(G^R)^{-1}(\omega \to 0)$ in the representation Eq. (45) without directly refering to an extended Hilbert space.

B. Dyson equation in second order in the electric field, electron scattering rate

We consider Eq. (44) to derive the first and second order expression for the Green's function G. The first order response to the perturbation M is obtained from $g_{0,1}$, which is an example of how to reproduce results from standard equilibrium theory (Kubo's linear response expression) from Keldysh Green's functions. To next (quadratic) order in Σ, we obtain the $N = 0$ (time averaged component) $G(\omega, N = 0)$ from

$$
g_{0,0} = g_0^0 - g_0^0 \Sigma [g_2^0 + g_{-2}^0] \Sigma g_{0,0},
\tag{51}
$$

which can be written as

$$
\begin{aligned}
G(\omega, N = 0) &= \left[(G^0)^{-1}(\omega) - S(\omega) \right]^{-1} \\
S(\omega) &:= \frac{1}{4} W G^0(\omega + \Omega) W + (\Omega \to -\Omega).
\end{aligned}
\tag{52}
$$

Specializing to the retarded functions, Eq. (7), we find $G^R(\omega, N = 0) = [(G^{0,R})^{-1}(\omega) - S^R(\omega)]^{-1}$, where $S^R(\omega) := (1/4) M G^{0,R}(\omega + \Omega) M + (\Omega \to -\Omega)$.

The determination of the Green's function Eq. (52) requires a full matrix inversion since S in general is a non-diagonal matrix. The diagonal part of the imaginary part of the retarded self energy $\operatorname{Im} S_{\alpha\alpha}^R$, however, has adirect physical meaning of an inverse lifetime of the state α. It describes the scattering rate for scattering out of state α to any other eigenstate of the system due to the perturbation. This quantity can be expressed exactly by

the real part $\mathrm{Re}\,\sigma_l(\varepsilon = \varepsilon_F, \Omega)$ of the AC conductivity as a function of the Fermi energy ε_F and frequency Ω *in absence* of the time-dependent perturbation $\mathbf{E}_0(t)$. In the limit of zero temperature $T = 0$, the derivation given in App. A yields

$$\tau_{MW}^{-1} = \tau_+^{-1} + \tau_-^{-1}, \quad \tau_\pm^{-1}(\varepsilon) = \frac{1}{2}\frac{E_0^2 \mathrm{Re}\,\sigma_l(\varepsilon \pm \hbar\Omega/2, \Omega)}{(\hbar\Omega)^2 \rho(\varepsilon)} + O\left(\frac{\hbar\Omega}{\varepsilon}\right)^2, \quad T = 0, \qquad (53)$$

where we reinstalled the $\hbar$ and $\rho(\varepsilon)$ denotes the density of states. This equation relates a physical quantity (the scattering time $\tau_\pm$) of the non-equilibrium system (static potential + electric field) to a linear transport-quantity of the equilibrium system (no electric field). The validity of this relation is independent of the eigenstate basis and in particular non-perturbative in the impurity potential. Basically, the reason why both quantities can be related to each other is that both essentially are given by the square of the matrix element of the velocity operator. It is also obvious why the (Fermi) energy ε is shifted by $\pm\hbar\Omega/2$ in the argument of the conductivity. The latter is due to particle hole excitations that lie symmetrically around the Fermi level ε, whereas $\tau_\pm$ describes electron scattering from ε to $\varepsilon \pm \hbar\Omega$. Furthermore, the expression for τ_{MW}^{-1}, Eq. (53), is valid for a single electron ('empty band'), i.e. no Pauli block by the other electrons. If the Fermi sea of the other electrons is considered, only scattering through photon absorption (+) is possible at zero temperature, and $\tau_{MW}^{-1} = \tau_+^{-1}$.

The physical meaning of Eq. (53) becomes particularily transparent by recalling that the *power* P_Ω absorbed by electrons subject to a homogeneous electric field E_0 is given by

$$P_\Omega(\varepsilon) = (1/2)E_0^2 \mathrm{Re}\,\sigma_l(\varepsilon) \cdot L^d, \qquad (54)$$

where L^d is the system volume. For frequencies Ω such that $\hbar\Omega \ll \varepsilon$, one can set $\varepsilon \pm \hbar\Omega \approx \varepsilon$, and Eq. (53) can be written

$$\frac{P_\Omega(\varepsilon)}{\hbar\Omega} = \frac{\hbar\Omega}{\Delta(\varepsilon)}\tau_+^{-1}(\varepsilon) = \rho(\varepsilon)(L^d\hbar\Omega)\,\tau_+^{-1}(\varepsilon), \qquad (55)$$

where $\Delta(\varepsilon) := (L^d\rho(\varepsilon))^{-1}$ is the mean level spacing at the energy ε. The number of photons absorbed per time, $P_\Omega(\varepsilon)/\hbar\Omega$, is given by the scattering rate, multiplied with the density of electronic states $\rho(\varepsilon)$ on the scale of the photon density of states $(L^d\hbar\Omega)^{-1}$.

C. Microwave radiation in the integer quantum Hall effect (IQHE)

As mentioned in the introduction, in the integer quantum Hall regime, microwave induced deviations $\Delta R_{xx}, \Delta R_{xy}$ of the resistance tensor have been observed experimentally [6]. One main finding was that these deviations are proportional to the square root of the incident microwave power, i.e. linear in the electric field amplitude E_0.

We calculated the microwave induced scattering rate Eq. (53) and found that this linear dependence *cannot* be explained in a simple scaling picture through the interplay of localization length and inelastic length. In fact, in the past the standard scaling picture of the IQHE [18] has been widely used to describe the scaling of the temperature (T)–dependent slope $(d\rho_{xy}/dB)^{max}$ and the inverse of the half- width of the $\rho_{xx}(B)$–peaks [19–21], i.e.

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temperature–dependent deviations $\Delta R_{xx/xy}$. The main idea is that the IQHE as a metal-insulator transition can be described in terms of a scaling function, depending on the ratio ξ/L_{in}, where ξ is the localization length and

$$L_{in} = (D\tau)^{1/2} \tag{56}$$

is a T–dependent inelastic length scale due to electron-electron and/or electron-phonon scattering at a rate τ^{-1}. D is a diffusion constant.

Although it is tempting to use this picture under inclusion of the additional inelastic scattering process due to the microwave, we found that such an explanation definitely is *not* appropriate. Our argument is as follows. At low temperatures, electron–electron scattering is believed to be dominant; in presence of microwave radiation, however, the scattering described by the rate Eq. (53) also should contribute. If the scattering due to the microwave is the main inelastic process, $\tau_{MW}^{-1} \gg \tau_{ee}^{-1}$, where τ_{ee}^{-1} stands for the rate due to electron–electron, and τ_{MW}^{-1} for the scattering by the time-dependent field, Eq. (53). One then has $L_{in} \approx (D\tau_{MW})^{1/2}$ in Eq. (56), and the scaling variable $\xi/L_{in} \sim E_0$ becomes proportional to the amplitude E_0 of the microwave field which would hint to the *linear* E_0– dependence of $\Delta R_{xx/xy}$. On the other hand, the electron-electron scattering is dominant for $\tau_{ee}^{-1} \gg \tau_{MW}^{-1}$. Estimating the effect by the microwave by adding the scattering *rates*, $\tau^{-1} = \tau_{ee}^{-1} + \tau_{MW}^{-1}$, one finds in this case

$$\tau^{-1} = \tau_{ee}^{-1}\left(1 + O(E_0^2)\right). \tag{57}$$

In particular this would mean that the (small) correction to the scaling variable due to the microwave radiation is *quadratic* in the amplitude E_0, and so should be any deviation to the resistance $R_{xx/xy}$.

We used the parameters of the experiment [6], Eq. (53), and a previous calculation of the rate τ_{ee}^{-1} [22] to compare both quantities. It turns out, that for temperatures $T \approx 0.5K$, $\Omega = 40Ghz$, $E_0 \approx 10^2 V/m$, the rate τ_{MW}^{-1} is orders of magnitudes smaller than the electron-electron scattering rate $\tau_{ee}^{-1} = \gamma k_B T/\hbar$ [22], where γ is a factor of order unity. Numerically, we find values approximately as $\tau_{ee}^{-1} \approx 10^{11} s^{-1}$ and $\tau_{MW}^{-1} \approx 10^8 s^{-1}$ for an estimated (small) conductivity $\sigma_{xx} \approx 10^{-2} e^2/h$. Even for a conductivity σ_{xx} close to the 'ideal' value $0.5 e^2/h$, the rate τ_{MW}^{-1} stays an order of magnitude behind the electron– electron scattering rate, and Eq. (57) should apply. This, in turn, is in contrast to the experimental finding $\Delta R \sim E_0$. From this negative result we conclude that an interpretation of the experimental data [6] is *not* possible in the above picture, simply using scaling arguments in combination with inelastic scattering rates. We believe that one has to go beyond an explanation that only makes use of scattering rates, i.e. the diagonal part of the self energy. Rather, one should start from the full Green's function Eq. (49) and investigate directly how quantities like the localization length are affected by the time dependent perturbation.

V. CONCLUSION

In this paper, we developed a method to calculate the Green's function of noninteracting electrons in static potentials in presence of time–dependent electric fields. The formalism was given in terms of Keldysh matrices (which are block–diagonal for static scattering).

Although not discussed here, in principal it allows inclusion of interaction processes in form of a suitable self energy for electron–electron or electron–phonon interactions.

In the first approach, by a double Fourier expansion a systematic perturbation was developed which is exact in the electric field and sums up the static potential to infinite order. Numerical examples for a constant and a simple double barrier potential showed that a few Fourier components already are sufficient to obtain convergence. We furthermore showed that this 'truncation method' is a systematic expansion around a non–adiabatic limit of high frequencies Ω of the electric field.

A second approach was given in the basis of the exact scattering states. There, the truncation method is a perturbation theory in the electric field which was explicitly shown for the self energy to second order. The latter was used to derive a relation between the rate for (inelastic) scattering induced by the time dependent field, and the AC conductivity in absence of the field. Application to microwave experiments in the integer Quantum Hall effect suggested, however, that rather than the microwave scattering rate the full Green's function in the basis of the scattering states has to be investigated.

Although in both methods exact solutions were derived, the numerical applicability suggests that the first approach is appropriate for relatively simple static potentials and strong electric fields. The second should be used for arbitrary (e.g. random) potentials but rather weak electric fields. Although the second approach has not yet been tested numerically, we propose to apply it to the localization–delocalization problem.

REFERENCES

[1] P. Hänggi (for a short review), in *ICTP–NATO Workshop on Quantum Dynamics*, Vol. 291 of *Nato ASI Series*, edited by H. Cerdeira, B. Kramer and G. Schön (Kluwer Academic Publishers, Dordrecht/Boston/London, 1994), p. 673.

[2] M. Wagner, Phys. Rev. Lett. **76**, 4010 (1996).

[3] R. Aguado, J. Iñarrea, and G. Platero, Phys. Rev. B **53**, 10030 (1996).

[4] L. P. Kouwenhoven *et al.*, Phys. Rev. B **50**, 2019 (1994).

[5] C. Bruder and H. Schoeller, Phys. Rev. Lett. **72**, 1076 (1994).

[6] R. Meisels, F. Kuchar, J. J. Harris, and C. T. Foxon, Surface Science **263**, 76 (1992).

[7] G. M. Sundaram *et al.*, in *ICTP–NATO Workshop on Quantum Dynamics*, Vol. 291 of *Nato ASI Series*, edited by H. Cerdeira, B. Kramer and G. Schön (Kluwer Academic Publishers, Dordrecht/Boston/London, 1994), p. 371.

[8] R. Meisels *et al.*, in *NATO Advanced Study Institute, Bad Lauterberg*, Vol. 326 of *Nata ASI Series E*, edited by B. Kramer (Kluwer Academic Publishers, Dordrecht, 1996).

[9] S. Feng and Q. Hu, Phys. Rev. B **48**, 5354 (1993).

[10] T. Brandes, Europhys. Lett. **33**, 629 (1996).

[11] M. Holthaus and D. W. Hone, Philosophical Magazine B **74**, 105 (1996).

[12] J. Iñarrea, G. Platero, and C. Tejedor, Phys. Rev. B **50**, 4581 (1994).

[13] G. D. Mahan, *Many–Particle Physics* (Plenum Press, New York, 1990).

[14] E. M. Lifshitz and L. P. Pitaevskii, *Physical Kinetics*, Vol. 10 of *Landau and Lifshitz, Course of Theoretical Physics* (Pergamon Press, Oxford, New York, 1981).

[15] R. Bertoncini and A. P. Jauho, Phys. Rev. B **44**, 3655 (1991).

[16] A. P. Jauho and K. Johnsen, Phys. Rev. Lett. **76**, 4576 (1996).

[17] J. H. Shirley, Phys. Rev. **138**, B979 (1965).

[18] A. M. M. Pruisken, Phys. Rev. Lett. **61**, 1297 (1988).

[19] H. P. Wei, D. C. Tsui, M. Paalanen, and A. M. M. Pruisken, Phys. Rev. Lett. **61**, 1294 (1988).

[20] S. Koch, R. J. Haug, K. v. Klitzing, and K. Ploog, Phys. Rev. Lett. **67**, 883 (1991).

[21] T. Brandes, L. Schweitzer, and B. Kramer, Phys. Rev. Lett. **72**, 3582 (1994).

[22] T. Brandes, Phys. Rev. B **52**, 8391 (1995).

APPENDIX A: DERIVATION OF THE SCATTERING RATE τ_{MW}^{-1}

Here, we derive the expression Eq. (53) for the inverse lifetime of a state α due to the time dependent electric field. First, the unperturbed Green's function is $G_{\alpha\beta}^{0,R}(\omega) = \delta_{\alpha\beta}(\omega - \varepsilon_\alpha + i0^+)^{-1}$. Note that energies are counted from zero and not from a chemical potential here. The coupling matrix element to the electric field is $M_{\alpha\beta} = (E_0/\Omega)\langle\alpha|v|\beta\rangle$, v is the component of the velocity operator in direction of the electric field polarization. This yields

$$
\begin{aligned}
\operatorname{Im} S_{\alpha\beta}^R(\omega) &\equiv \operatorname{Im} S_{\alpha\beta}^{R+}(\omega) + \operatorname{Im} S_{\alpha\beta}^{R-}(\omega) \\
&= -\pi\frac{E_0^2}{4\Omega^2}\sum_\gamma \langle\alpha|v|\gamma\rangle\langle\gamma|v|\beta\rangle\delta(\omega - \varepsilon_\gamma + \Omega) + (\Omega \to -\Omega),
\end{aligned} \tag{A1}
$$

where we defined the components corresponding to photon absorption $(+\Omega)$ and emission $(-\Omega)$ in Eq. (A1).

We now recall the expression for the real part of the longitudinal AC conductivity in linear response to an arbitrary homogeneous electric field of frequency Ω, namely in the zero-temperature limit

$$\mathrm{Re}\,\sigma_l(\varepsilon_F, \Omega) = \frac{\pi}{L^d} \sum_{\alpha\beta} |\langle\alpha|v|\beta\rangle|^2 \delta(\varepsilon_F + \Omega/2 - \varepsilon_\beta)\delta(\varepsilon_F - \Omega/2 - \varepsilon_\alpha) + O\left(\frac{\Omega}{\varepsilon_F}\right)^2. \qquad (A2)$$

We explicitly indicate the dependence of σ_l on the Fermi energy, furthermore v is the component of the velocity operator in one fixed direction, say v_x for σ_{xx}. We assume equality of all diagonal components of the conductivity tensor and the limit of zero temperature; note that the expression explicitly implies symmetry in Ω as it must be since $\mathrm{Re}\,\sigma_l(\varepsilon_F, \Omega) = \mathrm{Re}\,\sigma_l(\varepsilon_F, -\Omega)$.

The rate for scattering out of a state α with energy $\varepsilon = \varepsilon_\alpha$ due to photon absorption $(+)$ or emission $(-)$ is given by the diagonal part of the self energy,

$$\tau_{MW}^{-1} = \tau_+^{-1} + \tau_-^{-1}, \quad \tau_\pm^{-1}(\varepsilon) = -2\mathrm{Im}\,S_{\alpha\alpha}^{R\pm}(\varepsilon = \varepsilon_\alpha). \qquad (A3)$$

The relation between τ_{MW}^{-1} and the self energy S^R is as in the equilibrium case and can be directly verified by calculating the transition probability from a state α to a state β due to the time-dependent potential $M(t)$ as in the derivation of Fermi's 'golden rule'.

We assume that the diagonal elements of S^R depend on the quantum number α only through the corresponding eigenenergy ε_α. In particular, for a (spin-polarized) disorder broadened Landau band discussed below, there is a one-to-one correspondence of eigenstates and eigenenergies. From Eq. (A2), one finds

$$\mathrm{Re}\,\sigma_l(\varepsilon_F \pm \Omega/2, \Omega) = \pi\rho(\varepsilon_F) \sum_\beta |\langle\alpha|v|\beta\rangle|^2 \delta(\varepsilon_F \pm \Omega - \varepsilon_\beta)\Big|_{\varepsilon_\alpha = \varepsilon_F}, \qquad (A4)$$

where $\rho(\varepsilon) = (1/L^d) \sum_\alpha \delta(\varepsilon - \varepsilon_\alpha)$ is the density of states. Combining Eq. (A1), Eq. (A3), and Eq. (A4), one obtains Eq. (53).
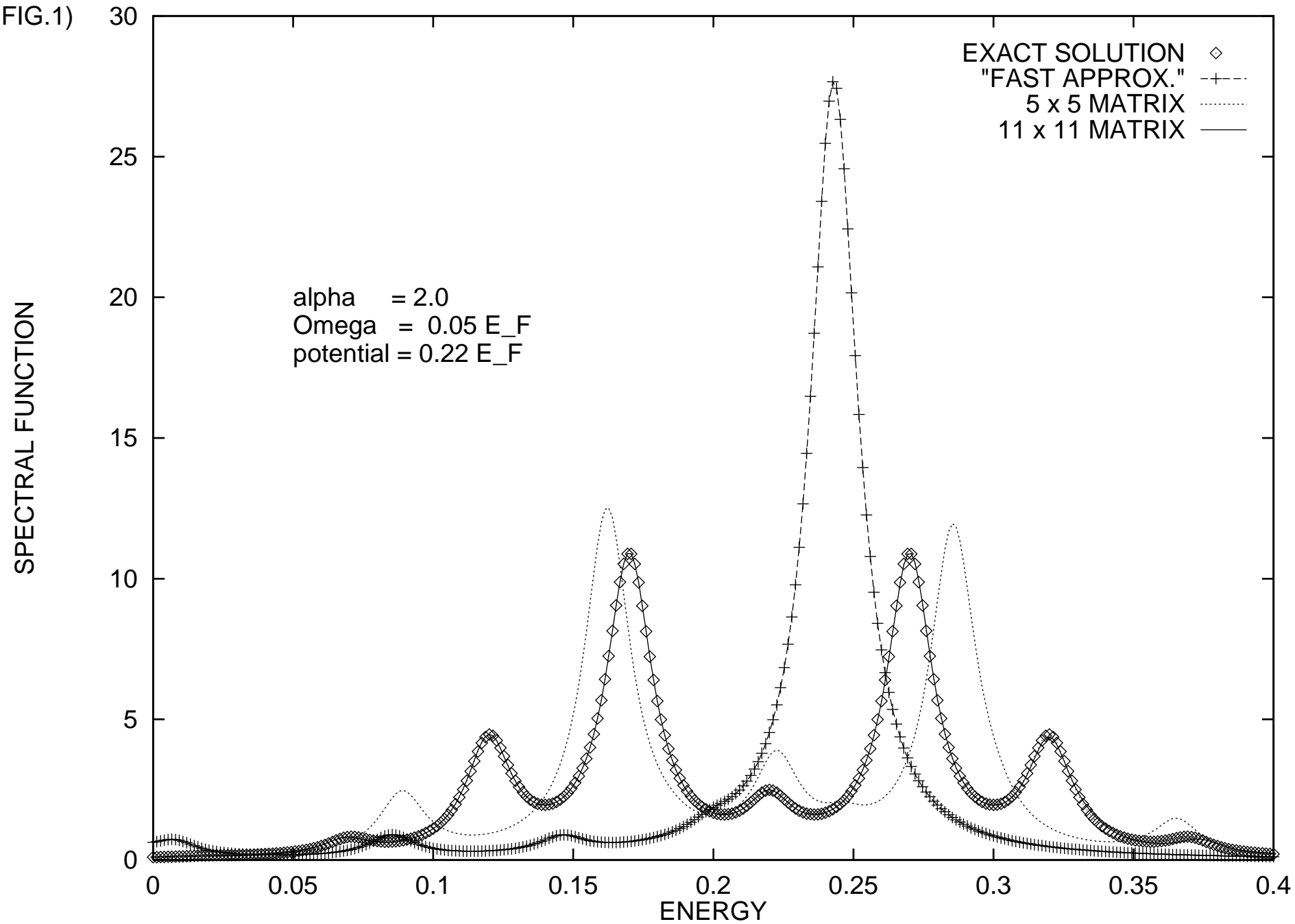
FIGURES

FIG. 1. The $N = 0$ spectral function component Eq. (35) in units of the inverse Fermi energy E_F^{-1} at the Fermi wave vector $k = k_F$. The model system describes a constant potential V and a time-dependent electric field of frequency Ω. The dimensionless parameter α regulates the coupling to the electric field, energies are in units of E_F. The exact solution is shown together with the result from the 'fast approximation', Eq. (28), and the result from the numerical inversion of Eq. (33). Already for $n_{ph} = 11$, practically for all energies coincidence is reached with the exact result Eq. (34).
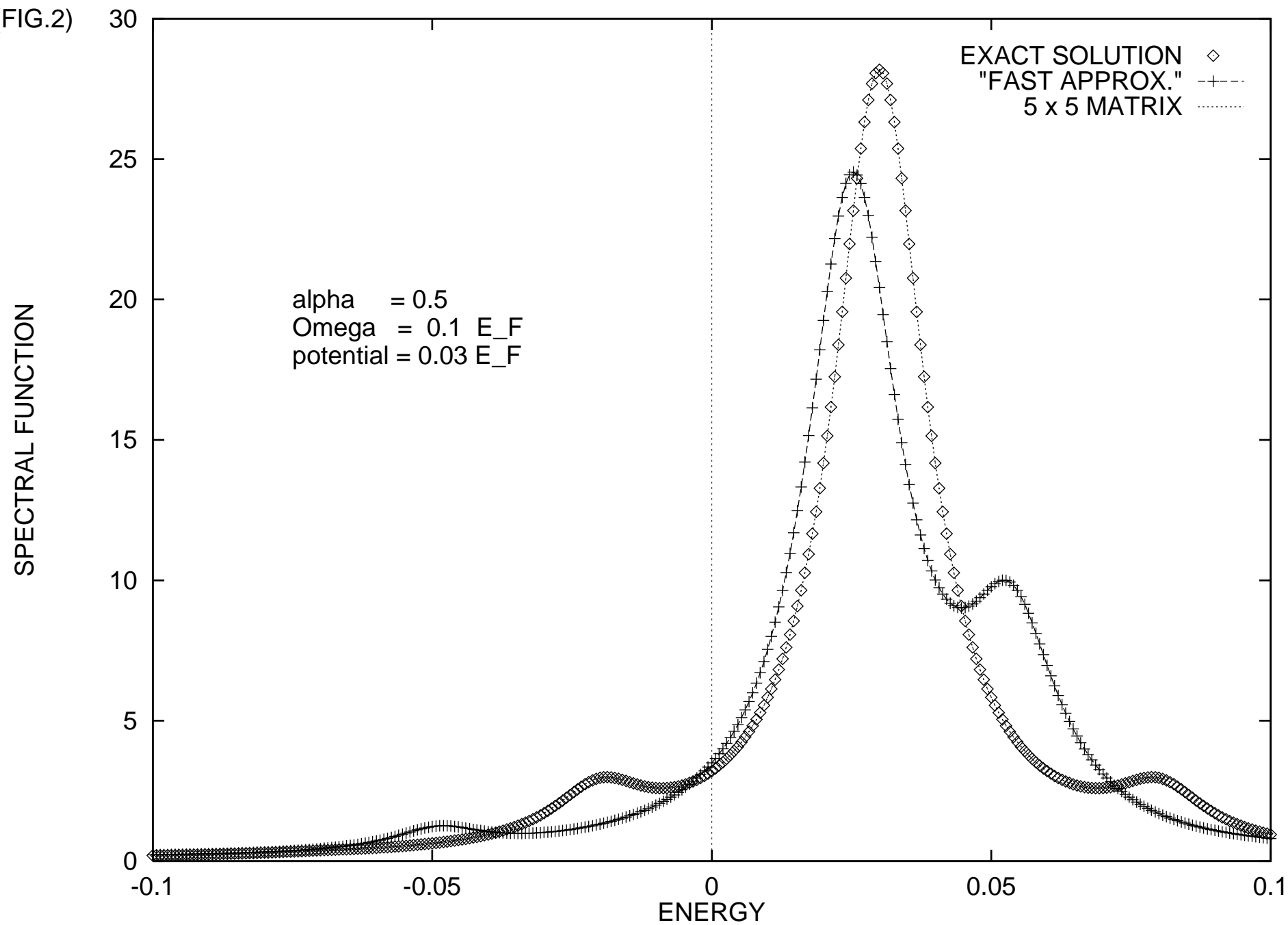
FIG. 2. Same as in Fig. (1) but for weaker coupling α and smaller potential V. Coincidence is reached for an even smaller matrix Eq. (33) in this case.

FIG. 3. Transmission coefficient Eq. (40) through a one-dimensional double barrier model in a time-dependent electric field with frequency Ω and coupling parameter α. Again, the Green's function has been calculated numerically for different numbers n_{ph} of 'photoblocks' in order to check the convergence of the results from inverting the truncated matrices Eq. (33). The system is defined by a 1d tight-binding model with 12 sites. The distance of the two potentials of strength $V = 20E_a$ defining the barrier is $2a$ with a the lattice constant; energies are in units of $E_a \equiv \hbar^2/2m^*a^2$. Site peaks in the transmission coefficient occur a energies shifted by $\pm\hbar\Omega$ from the central transmission peak.

(FIG.1)

EXACT SOLUTION ◇
"FAST APPROX." +---+---
5 x 5 MATRIX ·········
11 x 11 MATRIX ———

alpha   = 2.0
Omega   = 0.05 E_F
potential = 0.22 E_F

SPECTRAL FUNCTION

ENERGY

(FIG.2)

SPECTRAL FUNCTION

ENERGY

EXACT SOLUTION ◇
"FAST APPROX." +---
5 x 5 MATRIX ....

alpha   = 0.5
Omega   = 0.1 E_F
potential = 0.03 E_F

(FIG.3)